

# Impurity clusters and localization of nodal quasiparticles in $d$ -wave superconductors

Yu.G. Pogorelov

*IFIMUP/Departamento de Física, Universidade do Porto,  
R. Campo Alegre, 687, Porto, 4169-007, Portugal*

M.C. Santos

*Departamento de Física, Universidade de Coimbra, R. Larga, Coimbra, 3004-535, Portugal*

and V.M. Loktev

*Bogolyubov Institute for Theoretical Physics, 14b Metrologichna str., 03143 Kiev, Ukraine*

The long disputed issue of the limiting value of quasiparticle density of states  $\rho(0) = \rho(\varepsilon \rightarrow 0)$  in a  $d$ -wave superconductor with impurities (*vs* its linear vanishing,  $\rho_0(\varepsilon) \propto |\varepsilon|/\Delta$ , near the nodal point  $\varepsilon = 0$  in a pure system with the gap parameter  $\Delta$ ) is discussed. Using the technique of group expansions of Green functions in complexes of interacting impurities, it is shown that finite  $\rho(0)$  value is possible if the (finite) impurity perturbation  $V$  is spin-dependent (magnetic). The found value has a power law dependence on the impurity concentration  $c$ :  $\rho(0) \propto \rho_N c^n$ , where  $\rho_N$  is the normal metal density of states and  $n \geq 2$  is the least number of impurities in a complex that can localize nodal quasiparticle. This result essentially differs from the known predictions of self-consistent approximation:  $\rho(0) \propto \rho_N \sqrt{c/\rho_N \Delta}$  (for the unitary limit  $V \rightarrow \infty$ ) or  $\rho(0) \propto (\Delta/cV^2) \exp(-\Delta/cV^2 \rho_N)$  (for the Born limit  $|V|\rho_N \ll 1$ ). We predict also existence of a narrow interval (mobility gap) around the Fermi energy, where all the states are localized on proper impurity clusters, leading to exponential suppression of low-temperature kinetics.

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## INTRODUCTION

Key objects for the low-temperature physics of high- $T_c$  superconductors with planar lattice structure and  $d$ -wave superconducting (SC) order are quasiparticles of low energy,  $\varepsilon \ll \Delta \ll \varepsilon_F$  (where  $\Delta$  is the SC gap parameter and  $\varepsilon_F$  is the Fermi energy). In a clean  $d$ -wave system, they have “conical” energy dispersion:  $\varepsilon_{\mathbf{k}} \approx \hbar \sqrt{v_F^2 q_1^2 + v_\Delta^2 q_2^2}$ , if the wave vector  $\mathbf{k}$  is close to the nodal points  $\mathbf{k}_j$  ( $|\mathbf{k}_j| = k_F$ ,  $j = 1, \dots, 4$ , Fig. 1) on the Fermi surface. Here  $q_1$  and  $q_2$  are the radial and tangential components of the relative quasimomentum  $\mathbf{q} = \mathbf{k} - \mathbf{k}_j$  and the “gap” velocity  $v_\Delta$  is small beside the common Fermi velocity  $v_F$ :  $v_\Delta/v_F = \Delta/\varepsilon_F = \beta \ll 1$ . This defines the linear energy dependence of quasiparticle density of states (DOS):  $\rho_0(\varepsilon) \approx \rho_N |\varepsilon|/\Delta$  ( $\rho_N$  is the normal metal DOS), and respective power laws in temperature for thermodynamical quantities, in agreement with experimental data [1].

But this “clean” picture can fail at the lowest temperatures, dominated by the lowest energy excitations. By many analogies in the condensed matter, such excitations are expected to be the most sensitive to presence of impurities (almost inevitable in high- $T_c$  compounds). In particular, impurities can produce low energy resonances in the  $d$ -wave materials [2, 3], and even the possibility for impurity localization of quasiparticles was discussed [2, 4]. Traditionally, such effects were treated using certain forms of single-impurity approximation, as T-matrix approximation [5] or its generalization to the self-consistent T-matrix approximation (SCTMA) [6, 7].

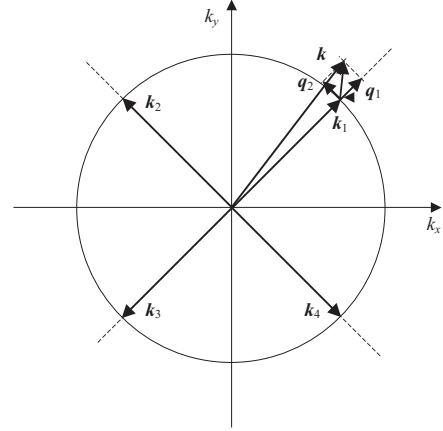


FIG. 1: Schematic of local coordinates near nodal points in the Brillouin zone of a  $d$ -wave superconductor.

Then, within the SCTMA scope, a finite limiting value of DOS,  $\rho(0) = \lim_{\varepsilon \rightarrow 0} \rho(\varepsilon)$ , was predicted either in the Born limit,  $|V|\rho_N \ll 1$  [8], and in the unitary limit,  $|V|\rho_N \gg 1$  [4, 6], for impurity perturbation  $V$ . However it was shown later that, for a properly defined SCTMA solution,  $\rho(0)$  should vanish (at any finite  $V$ ) [9]. The issue of finite or zero limit for DOS is of crucial importance for low temperature physics of real high- $T_c$  sys-

tems. Thus, supposing existence of  $\rho(0) \neq 0$ , P.A. Lee arrived at the prediction that the quasiparticle electric a.c. conductivity  $\sigma(\omega)$  in the static limit  $\omega \rightarrow 0$  should tend to a *universal* value  $\sigma(0) = (e^2/\pi^2\hbar\beta)$  [4], independent of impurity parameters at all! Similarly, a universal limit was predicted for the ratio of thermal conductivity to temperature,  $(\kappa/T)_{T \rightarrow 0} \rightarrow [nk_B^2/(3\hbar v_F v_\Delta d)](\beta^{-1} + \beta)$  [10, 11] (where  $n$  is the number of conducting planes per unit cell and  $d$  the distance between them). But no such behavior would be possible for the above referred alternative of vanishing DOS at  $\varepsilon \rightarrow 0$ . This alternative was predicted in various analytical forms: sublinear  $\rho(\varepsilon) \propto |\varepsilon|^\zeta$  with  $\zeta < 1$  [12] (also concluded from numerical solution of Bogolyubov-de Gennes equations [13]), linear  $\rho(\varepsilon) \propto |\varepsilon|$  (for non-magnetic impurities) [14], or superlinear  $\rho(\varepsilon) \propto \varepsilon^2$  (for magnetic impurities) [14] and  $\rho(\varepsilon) \propto |\varepsilon|/\ln^2(\Delta/|\varepsilon|)$  [15]. It should be also mentioned that some field theory approaches to this problem even resulted in diverging DOS:  $\rho(\varepsilon) \propto 1/|\varepsilon|\ln^2(\Delta/\varepsilon)$  [16] or  $\rho(\varepsilon) \propto \exp[A\sqrt{\ln(\Delta/\varepsilon)}]/|\varepsilon|$  [17]. Up to the moment, the experimental checks for universal behavior in the low-frequency electric transport [18, 19] and low-temperature heat transport [20, 21] do not provided a definitive support for any of these scenarios.

It is important to notice that either the SCTMA approach of Refs. [4, 11, 15] and the field-theory models of Refs. [12, 14, 17] are only justified if the relevant quasiparticle states are extended (non-localized). This requires that a quasiparticle with wavevector  $\mathbf{k}$  have the mean free path  $\ell$  longer than its wavelength  $\lambda = 2\pi/k$ , as expressed by the known Ioffe-Regel-Mott (IRM) criterion [22]. Also the derivation of the above mentioned universal limits fully relies on the Kubo formula integrals over the *extended* states (involving a certain lifetime  $\tau = \ell/v$  for given quasiparticle velocity  $v$ ). But in presence of *localized* states, the concepts of mean free path and lifetime do not make sense for them, and the Kubo formula should be reconsidered for the corresponding range of the spectrum, e.g., as for hopping transport in semiconductors [23]. Fortunately, the analysis of DOS can be done independently from the controversial issue of universal conductivity (postponing it for more detailed future treatment).

As to the limiting DOS values, it was shown [24] that the SCTMA approach in fact admits two solutions. One of them, called SCTMA-1, leads to finite  $\rho(0) \neq 0$  as given in Refs. [4, 8], but the other solution, SCTMA-2, yields in vanishing  $\rho(\varepsilon \rightarrow 0) \rightarrow |\varepsilon|/\ln^2(\Delta/|\varepsilon|)$ . And only SCTMA-2 proves to satisfy the IRM criterion at  $\varepsilon \rightarrow 0$ , thus appearing as the only valid SCTMA solution in this limit. Applying the same check to the power law solutions  $\rho(\varepsilon) \propto |\varepsilon|^\zeta$ , one finds them to satisfy the IRM criterion only if  $\zeta > 1$ , which is not actually the case in Refs. [12, 13] and [14] (for non-magnetic impurities). Thus, it could be thought that the ambiguity is resolved

in favor of the superlinearly vanishing SCTMA-2 DOS.

However the SCTMA (or field-theoretical) analysis can not be considered fully comprehensive for the real quasiparticle spectrum in a disordered system, if the localized states are also admitted. A more complete description is possible, noting that the SCTMA self-energy is only the first term of the so-called group expansion (GE) [15], where this term describes all the processes of quasiparticle scattering on *isolated* impurities. In accordance with the above IRM check, such processes can not produce localized states near zero energy. But if the SCTMA contribution to DOS vanishes in this limit, the importance can pass to the next terms of GE, related to scattering (and possible localization) of quasiparticles on random groups (clusters) of impurities. The essential point is that their contribution to DOS is mostly defined by the *real* parts of Green functions which do not need self-consistency corrections and thus remain valid for the energy range of localized states (where the IRM criterion does not hold).

The known approaches to impurity cluster effects in disordered  $d$ -wave superconductors, either numerical [25, 26] and analytical [16], were contradictory about DOS and did not conclude definitely on localization. A practical analysis of such effects within the GE framework for an  $s$ -wave superconductor was proposed recently [9], using a special algebraic technique in the limit  $\varepsilon \rightarrow \Delta$ . The present work develops a similar technique for a disordered  $d$ -wave system in the limit  $\varepsilon \rightarrow 0$ . We shall consider two main types of impurities, non-magnetic (NM) and magnetic (M), and show that only M-impurities can provide a finite (but different from the SCTMA-1 value) DOS, replacing the SCTMA-2 solution in a narrow vicinity of the (shifted) nodal energy and manifesting onset of localization there. The latter should produce, instead of universal conductivity, its exponential suppression at sufficiently low temperatures.

## FORMULATION OF PROBLEM

In more detail, we use the low energy Hamiltonian

$$H = \hbar \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger (v_F q_1 \hat{\tau}_3 + v_\Delta q_2 \hat{\tau}_1) \psi_{\mathbf{k}} + \frac{1}{N} \sum_{\mathbf{p}, \mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{p}} \psi_{\mathbf{k}}^\dagger \hat{V} \psi_{\mathbf{k}'} \quad (1)$$

where  $\mathbf{k}$  are restricted to vicinities of nodal points  $\mathbf{k}_j$ , the Nambu spinors  $\psi_{\mathbf{k}}^\dagger = (a_{\mathbf{k}}^\dagger, \alpha_{-\mathbf{k}})$  are composed of normal metal Fermi operators,  $N$  is the number of lattice sites and  $\hat{\tau}_i$  are Pauli matrices. The second term in Eq. 1 corresponds to the so called Lifshitz impurity model. It describes quasiparticle scattering on random sites  $\mathbf{p}$  with concentration  $c = \sum_{\mathbf{p}} 1/N \ll 1$  in lattice of  $N$  sites, and the perturbation matrix is:

$$\hat{V} = V \begin{cases} \hat{\tau}_3, & \text{NM,} \\ 1, & \text{M,} \end{cases} \quad (2)$$

for specific types of impurities. We calculate the Fourier transform of retarded Green function (GF) matrix

$$\left\langle \left\langle \psi_{\mathbf{k}} | \psi_{\mathbf{k}'}^\dagger \right\rangle \right\rangle_\varepsilon = i \int_0^\infty e^{i(\varepsilon + i0)t} \left\langle \left\{ \psi_{\mathbf{k}}, \psi_{\mathbf{k}'}^\dagger \right\} \right\rangle dt \quad (3)$$

where  $\langle \dots \rangle$  is the quantum-statistical average with the Hamiltonian, Eq. 1, and  $\{a, b\} = ab + ba$  is the anticommutator. The most important momentum-diagonal GF is presented as

$$\left\langle \left\langle \psi_{\mathbf{k}} | \psi_{\mathbf{k}}^\dagger \right\rangle \right\rangle_\varepsilon = (\hat{G}_{\mathbf{k}}^{-1} - \hat{\Sigma}_{\mathbf{k}})^{-1}, \quad (4)$$

where  $\hat{G}_{\mathbf{k}}(\varepsilon) = [\varepsilon + \hbar(v_F q_1 \hat{\tau}_3 + v_\Delta q_2 \hat{\tau}_1)] / (\varepsilon^2 - \varepsilon_{\mathbf{k}}^2)$  is the GF matrix of a clean system and the self-energy matrix  $\hat{\Sigma}_{\mathbf{k}}$  is expanded into the GE series [3]:

$$\hat{\Sigma}_{\mathbf{k}} = c\hat{T} \left[ 1 + c \sum_{\mathbf{n} \neq 0} \left( \hat{A}_{\mathbf{n}} \cos \mathbf{k} \cdot \mathbf{n} + \hat{A}_{\mathbf{n}}^2 \right) \times \left( 1 - \hat{A}_{\mathbf{n}}^2 \right)^{-1} + \dots \right]. \quad (5)$$

Here the T-matrix  $\hat{T}(\varepsilon) = \hat{V} (1 - \hat{G}\hat{V})^{-1}$ , with local GF matrix  $\hat{G}(\varepsilon) = N^{-1} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}}$ , describes all the scattering processes on a single impurity center. It can have resonance behavior near a certain energy  $\varepsilon_{res} < \Delta$ , such that  $\text{Re det} [1 - \hat{G}(\varepsilon_{res}) \hat{V}] = 0$  [2, 3, 9], however at  $\varepsilon \rightarrow 0$  it simply tends to a certain real matrix  $\hat{T}(0)$ , to be specified below.

The next to unity term in the brackets of Eq. 5 describes scattering on pairs of impurities, separated by all possible lattice vectors  $\mathbf{n}$ , while the dropped terms are for impurity triples and so on. The building block of all GE terms is the matrix  $\hat{A}_{\mathbf{n}}(\varepsilon) = N^{-1} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{n}} \hat{G}_{\mathbf{k}} \hat{T}$  which represents the effective (energy dependent) interaction between two impurities at given separation  $\mathbf{n}$ . Its zero energy limit is

$$\hat{A}_{\mathbf{n}}(0) = (g_{\mathbf{n}} \hat{\tau}_3 + f_{\mathbf{n}} \hat{\tau}_1) \hat{T}(0), \quad (6)$$

with real functions  $g_{\mathbf{n}} = -(\hbar v_F / N) \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{n}} q_1 / \varepsilon_{\mathbf{k}}^2$  and  $f_{\mathbf{n}} = -(\hbar v_\Delta / N) \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{n}} q_2 / \varepsilon_{\mathbf{k}}^2$ . Then the DOS reads:

$$\rho(\varepsilon) = \frac{1}{N\pi} \sum_{\mathbf{k}} \text{Im Tr} \left\langle \left\langle \psi_{\mathbf{k}} | \psi_{\mathbf{k}}^\dagger \right\rangle \right\rangle_\varepsilon, \quad (7)$$

and in absence of impurities it is  $\rho_0(\varepsilon) = \pi^{-1} \text{Im} g(\varepsilon)$ , where  $g(\varepsilon) = N^{-1} \text{Tr} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}} \approx (2\rho_N \varepsilon / \Delta) \ln(2i\Delta/\varepsilon)$  [15], vanishing linearly with  $\varepsilon \rightarrow 0$ . In presence of impurities, Eqs. 4 and 5 generally relate the limit  $\rho(\varepsilon \rightarrow 0)$  with the imaginary and traceful part of the self-energy matrix:  $\gamma = \frac{1}{2} \text{Tr Im} \hat{\Sigma}_{\mathbf{k}}(0)$ . If the main contribution to  $\gamma$  comes from the GE pair term, where the share of  $\hat{A}_{\mathbf{n}} \cos \mathbf{k} \cdot \mathbf{n}$  is negligible beside that of  $\hat{A}_{\mathbf{n}}^2$ ,  $\gamma$  can be considered momentum-independent. In this approximation, supposing also  $\gamma \ll \Delta$ , we obtain

$$\rho(0) \approx \rho_N \frac{2\gamma}{\pi\Delta} \ln \frac{\Delta}{\gamma} \ll \rho_N, \quad (8)$$

and the following task is reduced to proper calculation of  $\gamma$  in function of the impurity perturbation parameters.

Since the above mentioned matrices  $\hat{T}(0)$  and  $\hat{A}_{\mathbf{n}}$  are real, the imaginary part of the GE pair term is generated by the poles of  $(1 - \hat{A}_{\mathbf{n}}^2)^{-1}$ . If there is no such poles, one has to search for contributions to  $\gamma$  from next order GE terms. In this course, for an  $l$ th order GE term, the imaginary part is related to the poles of the inverse of a certain  $l$ th degree polynomial in  $\hat{A}_{\mathbf{n}}, \dots, \hat{A}_{\mathbf{n}_{l(l-1)/2}}$  (where  $\mathbf{n}_1, \dots, \mathbf{n}_{l(l-1)/2}$  are all possible separations between  $l$  impurities).

Generally, in the energy spectrum of a crystal with impurities, one can distinguish certain intervals where DOS is dominated by contributions from band-like states, single impurities, impurity pairs, triples, etc. [27]. Then, for instance, in the pair-dominated energy interval, each discrete peak (by an impurity pair at given separation  $\mathbf{n}$  in the lattice) experiences small shifts, due to the effects by neighbor impurities of such a pair, different in different parts of the system. These shifts produce a broadening of pair peaks, and if it is wider than the distance between the peaks, the resulting continuous pair-dominated spectrum can be effectively described, passing from summation in discrete  $\mathbf{n} \neq 0$  in Eq. 5 to integration in continuous  $\mathbf{r}$  (for  $r > r_0$  where  $r_0 \sim a$ ). Such possibility was shown long ago for normal electron spectrum [28], and it is even more pronounced for the superconducting system where the pair contribution to DOS at a given energy can come from multiple pair configurations (see Figs. 2,4 below) and this multiplicity turns yet much greater at involving neighbor impurities into each configuration. An approach to analogous problem in  $s$ -wave superconductors was proposed recently [9], using an algebraic isomorphism of the matrices of interaction between impurities in that system to common complex numbers.

## NON-MAGNETIC IMPURITIES

Remarkably, the same isomorphism is also found for matrices of zero energy interaction  $\hat{A}_{\mathbf{n}}$  between NM impurities in the  $d$ -wave system. In this case, we have

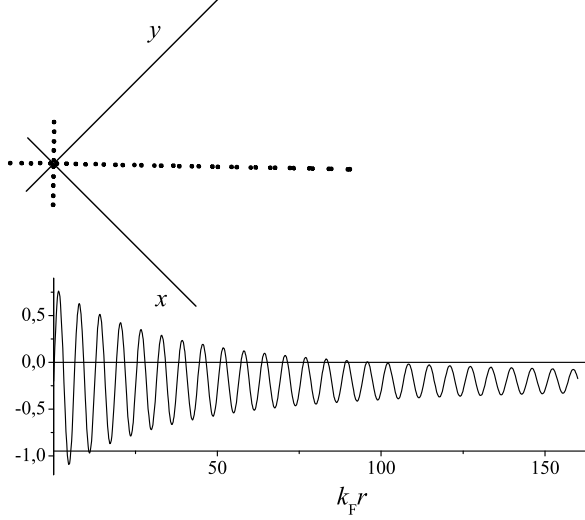


FIG. 2: The poles of the integrand in Eq. 9 in function of pair separation vector  $\mathbf{r} = (x, y)$ , are located along the nodal (the direct space), where one of the pole conditions,  $f_{\mathbf{r}} = 0$ , holds identically. Another pole condition,  $|g_{\mathbf{r}}| = 1/|\tilde{V}| = |g_{as} - 1/V|$ , is reached at discrete points (here at the choice of parameters  $\beta = 0.05$ ,  $\tilde{V}g_{as} = 5$ ). The plot below shows the related behavior of  $g_{\mathbf{r}} - 1/\tilde{V}$  for  $\mathbf{r}$  along the nodal direction.

explicitly:  $\hat{T}(0) = \tilde{V}\hat{\tau}_3$ , where  $\tilde{V} = V/(1 - Vg_{as})$  and  $g_{as} \approx \rho_N \ln|1/\rho_N\varepsilon_F - 1|$  is the factor of particle-hole asymmetry (away from half-filling:  $\rho_N\varepsilon_F \neq 1/2$ ). Then the interaction matrices, Eq. 6, are presented as  $\hat{A}_{\mathbf{n}} = \tilde{V}g_{\mathbf{n}} + i\tilde{V}f_{\mathbf{n}}\hat{\tau}_2$ , thus pertaining to the general two-parametric family  $\hat{C}(x, y) = x + iy\hat{\tau}_2$  with real  $x, y$ . This family forms an algebra with the product  $\hat{C}(x, y)\hat{C}(x', y') = \hat{C}(xx' - yy', xy' + xy')$ , isomorphic to that considered in Ref. [9] and to the algebra  $\mathbb{C}$  of common complex numbers:  $(x + iy)(x' + iy') = xx' - yy' + i(xy' + xy')$ . By this isomorphism, the real matrix  $\hat{A}_{\mathbf{n}}$  is related to a “complex number”  $A_{\mathbf{n}} = \tilde{V}g_{\mathbf{n}} + i\tilde{V}f_{\mathbf{n}}$ , where the “imaginary unity”  $\hat{i}$  corresponds to the real matrix  $\hat{i} \equiv i\hat{\tau}_2$ . Using such “complex” representation and the above mentioned passage from summation in  $\mathbf{n}$  to integration in  $\mathbf{r}$ , we can write the pair contribution to  $\gamma$  in the form:

$$c^2 \text{Im} \int_{r > r_0} \frac{d\mathbf{r}}{a^2} \Re \frac{p(\mathbf{r}) + \hat{i}q(\mathbf{r})}{s(\mathbf{r}) + \hat{i}t(\mathbf{r})}, \quad (9)$$

with  $s = 1 - \tilde{V}^2(g_{\mathbf{r}}^2 - f_{\mathbf{r}}^2)$ ,  $t = -2V^2g_{\mathbf{r}}f_{\mathbf{r}}$  and some continuous functions  $p(\mathbf{r}), q(\mathbf{r})$ . Here the symbol  $\Re$  means the “real” (traceful) part of the “complex” integrand, while the common imaginary part  $\text{Im}$  is produced by its poles. These are attained at such separations  $\mathbf{r} = \mathbf{r}^*$  of an impurity pair that  $s(\mathbf{r}^*) = t(\mathbf{r}^*) = 0$ , which requires

$|g_{\mathbf{r}^*}| = \tilde{V}^{-1}$  and  $f_{\mathbf{r}^*} = 0$ . Direct calculation of  $g_{\mathbf{r}}$  and  $f_{\mathbf{r}}$  shows that all possible  $\mathbf{r}^*$  lie on nodal directions, forming identical finite series along them (like those in Fig. 2). Also we note that poles only exist at high enough band filling,  $\rho_N\varepsilon_F \geq (1 + e)^{-1}$  and strong enough perturbation parameter,  $V \geq (\rho_N - g_{as})^{-1}$ , as chosen in Fig. 2. If so, it is suitable to pass in the vicinity of each  $\mathbf{r}^*$  from integration in the components  $r_1, r_2$  of vector  $\mathbf{r}$  to that in the components  $s, t$  of the “complex” denominator:

$$\text{Im} \sum_{\mathbf{r}^*} \int ds dt \mathcal{J}_{\mathbf{r}^*}(s, t) \frac{p(s, t)s + q(s, t)t}{s^2 + t^2}, \quad (10)$$

and for any  $\mathbf{r}^*$  the transformation Jacobian

$$\mathcal{J}_{\mathbf{r}^*}(s, t) = \left. \frac{\partial(r_1, r_2)}{\partial(s, t)} \right|_{\mathbf{r}=\mathbf{r}^*}$$

is real and non-singular. Then the singularity in the denominator of Eq. 10 is canceled by the vanishing residue in the numerator and, even at formal existence of poles in Eq. 9, they give no contribution to the zero energy DOS. Mathematically, this simply follows from an extra dimension at 2D integration, giving zero weight to the isolated poles.

The above conclusion can be immediately generalized for any  $l$ th order GE term ( $l \geq 3$ ), where the integrand is again presented as  $(p + \hat{i}q)/(s + \hat{i}t)$  and  $p, q, s, t$  are now continuous functions of  $N_l = 2(l - 1)$  independent variables (components of the vectors  $\mathbf{r}_1, \dots, \mathbf{r}_{l-1}$ ) in the configurational space  $\mathcal{S}_l$ . This integrand can have simple poles on some  $(N_l - 2)$ -dimensional surface  $\mathcal{A}_l$  in  $\mathcal{S}_l$  (under easier conditions than for  $l = 2$ ). Then the  $N_l$ -fold integration can be done over certain coordinates  $u_1, \dots, u_{N_l-2}$  in  $\mathcal{A}_l$  and over the components  $s, t$  of the “complex” denominator in the normal plane to  $\mathcal{A}_l$ :

$$\text{Im} \int du_1 \dots du_{N_l-2} \mathcal{J}(u_1, \dots, u_{N_l-2}) \times \int ds dt \frac{p(\dots, s, t)s + q(\dots, s, t)t}{s^2 + t^2}, \quad (11)$$

with a non-singular Jacobian  $\mathcal{J}$ . The latter integral has no imaginary part by the same reasons as for Eq. 10. Thus, it can be concluded that perturbation by NM-impurities in a  $d$ -wave system can not produce localized quasiparticles of zero energy, and this directly follows from the indicated isomorphism of the interaction matrices to the algebra  $\mathbb{C}$  of complex numbers.

Moreover, the same conclusion is also valid for yet another type of NM-perturbation, due to locally perturbed SC order by the matrix  $\hat{V} = V\hat{\tau}_1$ . In this case, the interaction matrix:

$$\hat{A}_{\mathbf{n}} = \frac{V}{1 - V^2g_{as}^2} [f_{\mathbf{n}} + Vg_{as}g_{\mathbf{n}} + i(g_{\mathbf{n}} - Vg_{as}f_{\mathbf{n}})\hat{\tau}_2],$$

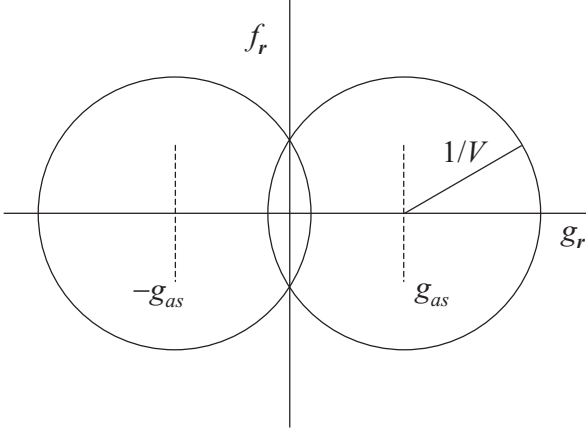


FIG. 3: Circular trajectories in the space of variables  $g_r, f_r$ , corresponding to the poles of GE denominator, Eq. 14, for M impurities at the choice of  $V = 1/\rho_N$  and  $g_{as} = 0.84\rho_N$ .

pertains to the same family  $\hat{C}(x, y)$  as in the above case, hence leading to the same absence of contribution to the zero energy DOS.

### MAGNETIC IMPURITIES

However, an essential cluster contribution to zero energy DOS can be produced by M impurities with the scalar (see Eq. 2) local perturbation  $\hat{V} = V$ , the respective T-matrix in the zero energy limit being:

$$\hat{T}(0) = V(1 - V\hat{G})^{-1} = V \frac{1 + Vg_{as}\hat{\tau}_3}{1 - V^2g_{as}^2}. \quad (12)$$

Unlike the traceless  $\hat{T}(0)$  for NM-impurities, this matrix produces a finite shift of the nodal point itself, from  $\varepsilon = 0$  to  $\varepsilon = \varepsilon_0 = cV(1 - V^2g_{as}^2)^{-1}$ . As usual, this can be absorbed into the Fermi level position by shifting all the energy arguments of considered GF's, then DOS in T-matrix (or SCTMA) approximation will vanish at  $\varepsilon \rightarrow \varepsilon_0$  (in the same way as at  $\varepsilon \rightarrow 0$  for NM-impurities), fixing the relevant limit in presence of M impurities. The following treatment of higher order GE terms involves the matrix of interaction between M-impurities:

$$\hat{A}_r = V \frac{(\hat{\tau}_3 + Vg_{as})g_r + (\hat{\tau}_1 - iVg_{as}\hat{\tau}_2)f_r}{1 - V^2g_{as}^2}. \quad (13)$$

Notably, it does not fit the  $\mathbb{C}$  algebra, and though being harder technically, this permits to expect that M-impurities can effectively contribute to the zero energy DOS. In fact, the straightforward calculation of the corresponding GE pair term leads to the general matrix expression

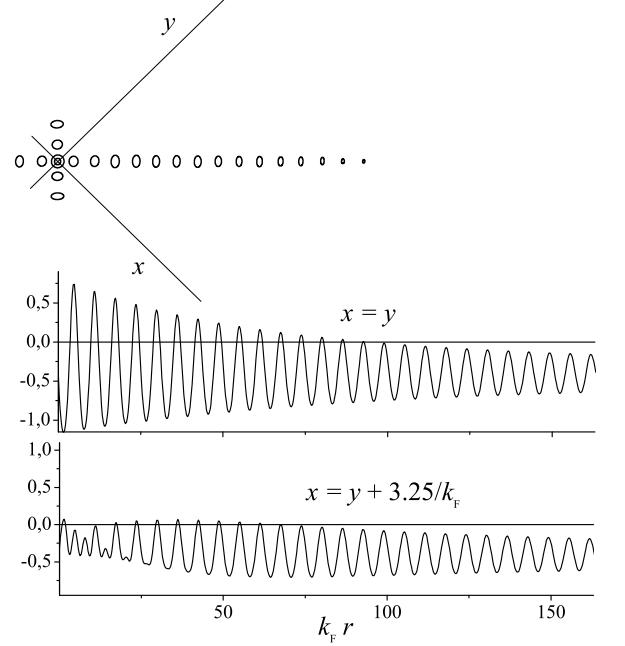


FIG. 4: In the  $\mathbf{r}$ -plane, the trajectories of zeroes of  $D_r$  form continuous loops within the stripes of  $\sim v_F/(v_\Delta|\delta|k_F)$  length and  $\sim 1/(|\delta|k_F)$  width along the nodal axes. The plots below present the pair GE term denominator  $D_r$  (at the same choice of parameters as in Fig. 3), seen along the stripe axis and along the stripe border.

$$(1 - \hat{A}_r^2)^{-1} = \frac{N_0 + N_1\hat{\tau}_1 + iN_2\hat{\tau}_2 + N_3\hat{\tau}_3}{D_r}. \quad (14)$$

Here  $N_j$ 's in the numerator are certain functions of  $g_r, f_r$  and the denominator  $D$  is the 4th grade polynomial:

$$D = \left[ f_r^2 + (g_r - g_{as})^2 - \frac{1}{V^2} \right] \left[ f_r^2 + (g_r + g_{as})^2 - \frac{1}{V^2} \right].$$

Zeroes of  $D$  in the space of variables  $g_r, f_r$  form two circular trajectories of radius  $1/V$  centered at  $\pm g_{as}$ , as shown in Fig. 3 (cf. to their location in the two outer points of these circles,  $f_r = 0, \pm g_r = g_{as} + 1/V$ , in the NM case). It is this extension of singularities, from isolated points to continuous trajectories, that allows finite imaginary part of the 2D integral

$$\gamma \approx \frac{c^2V}{1 - V^2g_{as}^2} \text{Im} \int \frac{d\mathbf{r}}{a^2} \frac{N_0 + Vg_{as}N_3}{D_r}. \quad (15)$$

On the other hand, it is assured by the fact that the traceful numerator  $N_0 + Vg_{as}N_3$  in Eq. 15 does not vanish on these trajectories. Quantitative analysis is simplified in the case of  $Vg_{as} \approx 1$ , when the small parameter

$\delta = 1 - V^2 g_{as}^2$  (such that  $|\delta| \ll 1$ ) defines a low energy resonance at  $\varepsilon_{res} \approx \Delta\delta/[V\rho_N \ln(1/\delta^2)]$  [29]. In this case we have simply  $N_0 + Vg_{as}N_3 \approx -2g_{\mathbf{r}}^2/V^2$ . Direct numeric calculation of the functions  $g_{\mathbf{r}}, f_{\mathbf{r}}$  shows that the trajectories  $D = 0$ , when presented in variables  $r_{1,2}$ , form multiple loops (seen in the inset of Fig. 4) of total number  $\sim v_F/(v_\Delta|\delta|)$ , each contributing by  $\sim \pi^2/[(ak_F)^2|\delta|]$  into  $\text{Im} \int g_{\mathbf{r}}^2/(V^2 D) d\mathbf{r}/a^2$  in Eq. 15. Thus we arrive at the estimate:  $\gamma \sim c^2 V/|\delta|$ , and hence to the finite residual DOS:

$$\rho(\varepsilon_0) \sim \rho_N \frac{c^2 V}{\Delta|\delta|} \ln \frac{\Delta|\delta|}{c^2 V}. \quad (16)$$

We recall that this result is impossible in the properly formulated self-consistent approximation [15], and it is also in a striking difference to the SCTMA predictions,  $\rho(0) \sim (\Delta/V^2 \rho_N) \exp(-\Delta/cV^2 \rho_N)$  in the Born limit [8] or  $\rho(0) \sim \sqrt{c\rho_N/\Delta}$  in the unitary limit [4]. The non-universality of this effect is manifested by its sensitivity to the M-perturbation parameter  $V$ , so that  $\rho(\varepsilon_0)$  is defined by impurity pairs only for strong enough perturbations,  $|V| \gtrsim (\rho_N + g_{as})^{-1}$ . For weaker  $V$ , nodal quasiparticles will be only localized on impurity clusters of a greater number  $n > 2$  (the bigger the smaller  $|V|$ ), and the particular form of Eq. 16 would change to  $\rho(0) \sim \rho_N c^n$  (with some logarithmic corrections). Anyhow, a finite limit of DOS at zero energy is granted by the fact that in real high- $T_c$  systems a certain M-type perturbation can result even from nominally non-magnetic centers (including dopants) [29]. Moreover, the above considered condition  $|V|g_{as} \approx 1$  does not seem very difficult, as testified by the observation of extremely low-energy resonance  $\varepsilon_{res} \approx -1.5$  meV by Zn impurities in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  [33]. It just fits the asymmetric M-resonance from Fig. 5, contrasting with the symmetric NM-resonance picture.

Then the overall impurity effect in a  $d$ -wave superconductor can be seen as a superposition (almost independent) of the above described effects from NM-impurities with perturbation parameter  $V_{NM}$  and concentration  $c_{NM}$  and from M-impurities with perturbation parameter  $V$  and concentration  $c$  (supposedly  $c \ll c_{NM}$ ). An example of such situation is shown in Fig. 5.

The residual DOS from pair GE term prevails within a certain narrow vicinity of  $\varepsilon_0$  where quasiparticle states are all localized on properly separated impurity pairs. Outside this vicinity, the states are extended and reasonably described by T-matrix (or SCTMA). The transition from localized to extended states occurs at the Mott mobility edges  $\varepsilon_c < \varepsilon_0$  and  $\varepsilon_{c'} > \varepsilon_0$ , where GE and T-matrix contributions to DOS are comparable. Using the simplest approximation for the T-matrix term:  $\rho(\varepsilon) \sim \rho_N |\varepsilon - \varepsilon_0|/\Delta$ , we estimate the range of localized states (somewhat exaggerated in the inset of Fig. 5) as

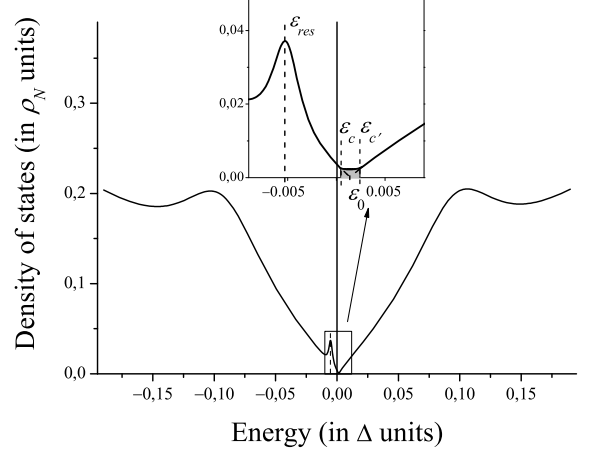


FIG. 5: Low-energy  $d$ -wave DOS  $\rho(\varepsilon)$  in simultaneous presence of NM-impurities (with  $c_{NM} = 3\%$  and  $V_{NM} = 1/\rho_N$ ), producing two symmetric broad resonances, and M-impurities (with  $c = 0.03\%$ ,  $V = V_{NM}$ , and  $Vg_{as} = 0.9$ ), producing single sharp resonance at extremely low energy  $\varepsilon_{res}$ . Inset shows the mobility edges  $\varepsilon_c$  and  $\varepsilon_{c'}$  around the shifted nodal point  $\varepsilon_0$ , they separate localized states (shaded area) with almost constant DOS,  $\rho(\varepsilon) \approx \rho(\varepsilon_0)$ , from band-like states whose DOS is close to the T-matrix value (solid line).

$$\varepsilon_{c'} - \varepsilon_0 \sim \varepsilon_0 - \varepsilon_c \sim \delta_c \sim \frac{c^2 V}{|\delta|} \ln \frac{\Delta|\delta|}{c^2 V}, \quad (17)$$

provided it is much smaller than the distance to the M-resonance:  $\delta_c \ll |\varepsilon_0 - \varepsilon_{res}|$ . The same estimates for the mobility edges follow from the IRM breakdown condition:  $\varepsilon - \text{Re}\Sigma(\varepsilon) \sim \text{Im}\Sigma(\varepsilon)$ , at  $\varepsilon \approx \varepsilon_0$ .

The tendency to localization of quasiparticles can be generally opposed by the effects of repulsive Coulomb interaction between them [30] and this issue was also discussed for disordered  $d$ -wave superconductors [17, 31]. These field theory treatments showed that localization can survive at low enough temperature. The full account of Coulomb interactions in the present GE approach is rather complicated technically, but a simple estimate follows from the overall number of (supposedly) localized particles within the energy range, Eq. 17, which is as small as  $n_{loc} \sim \rho(\varepsilon_0)\delta_c \sim (c^4 V/\Delta\delta^2) \ln^2 |\Delta\delta/c^2 V|$ . Since the average distance between them  $\sim a/\sqrt{n_{loc}}$  is much longer than the distance between charge carriers  $\sim a/\sqrt{n} \sim a/\sqrt{\rho_N \varepsilon_F}$ , the effects of Coulomb interaction are hopefully screened out, at least for the systems far enough from half-filling [32].

Notably, localization turns to be yet possible near the resonance energy,  $\varepsilon \approx \varepsilon_{res}$ , but this requires that the concentration of M-impurities surpasses a certain characteristic value  $c_{res} \sim (\varepsilon_{res}/\Delta)^2 \ln(\Delta/|\varepsilon_{res}|)$ . In par-

ticular, for the choice of parameters in Fig. 5, we find  $c_{res} \sim 3 \cdot 10^{-4}$ , so that this system should be close to the onset of localization also in this spectrum range, where each localized state is associated with a *single* impurity center.

Generally, presence of localized states near the lowest excitation energies in the spectrum must influence significantly the kinetic properties of a crystal with impurities, such as electric and (electronic part of) heat conductivity at lowest temperatures. Taking in mind the above referred modification of Kubo formula for the energy range  $|\varepsilon - \varepsilon_0| < \delta_c$ , their temperature dependencies, instead of reaching the universal values  $\sigma_0$  and  $[\kappa/T](0)$ , should rather tend to the exponential vanishing:  $\sim \exp(-\delta_c/k_B T)$ , at low enough temperatures:  $T \ll \delta_c/k_B$ . The latter value, at the same choice of impurity perturbation parameters and typical gap  $\Delta \sim 30$  meV, is estimated as  $\sim 0.2$  K. In this context, the intriguing sharp downturn of  $\kappa/T$ , recently observed at temperatures  $\lesssim 0.3$  K [34] and attributed to the low-temperature decoupling of phonon heat channel [35], can be otherwise considered as a possible experimental manifestation of the quasiparticle localization by impurity clusters. A more detailed analysis of possible non-universal behavior of transport properties of disordered *d*-wave superconductors will be necessary to confirm this conjecture.

## CONCLUSIONS

The quasiparticle states are considered in a *d*-wave superconductor with impurities beyond the (self-consistent) T-matrix approximation, using the techniques of group expansions of Green functions in complexes of interacting impurities. It is shown that, if the impurity perturbation of magnetic type is present, the indirect interaction between impurities can essentially change the quasiparticle spectrum near nodal points, producing strongly localized states of non-universal character (depending on the perturbation strength). Experimental check for possible non-universal effects in low temperature transport properties can be done, e.g., in the Zn doped  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  system.

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